

# Very large scale simulations of the RSOS model in four dimensions

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We study the Restricted Solid on Solid (RSOS) model for surface growth in spatial dimension  $d = 4$  by means of a *multi-surface coding* technique that allows to analyze samples of unprecedented size. For such large systems we are able to achieve a controlled asymptotic regime where the typical scale of the fluctuations are larger than the lattice spacing used in the simulations. A careful finite-size scaling analysis of the critical exponents clearly indicate that  $d = 4$  is not the upper critical dimension of the model.

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The Kardar-Parisi-Zhang (KPZ) equation [1] is possibly the simplest, most studied, and yet not fully understood model for out-of-equilibrium surface growth. The equation describes the time evolution of the height  $h(\mathbf{r}, t)$  of an interface above a  $d$ -dimensional substrate:

$$\partial_t h(\mathbf{r}, t) = \nu \bar{\nabla}^2 h(\mathbf{r}, t) + \frac{\lambda}{2} |\bar{\nabla} h(\mathbf{r}, t)|^2 + \eta(\mathbf{r}, t), \quad (1)$$

where  $\nu$  is the diffusion coefficient,  $\lambda$  is the strength of the non-linear growth rate term which is responsible for the  $h \rightarrow -h$  symmetry breaking with respect to the growing direction, and  $\eta(\mathbf{r}, t)$  is a Gaussian white noise of amplitude  $D$ :

$$\langle \eta \rangle = 0, \quad \langle \eta(\mathbf{r}, t) \eta(\mathbf{r}', t') \rangle = 2D \delta^d(\mathbf{r} - \mathbf{r}') \delta(t - t'). \quad (2)$$

The KPZ equation describe many relevant growth processes, such as the Eden model, ballistic deposition, interface growth in disordered medium. It is also related to many other physical phenomena apparently unrelated to surface growth, such as Burgers turbulence, dynamics directed polymers in random media, dissipative transport in the driven-diffusion equation [2].

The scaling properties of the height's fluctuations  $w_2(L, t) = \langle h^2(\mathbf{r}, t) \rangle_{\mathbf{r}} - \langle h(\mathbf{r}, t) \rangle_{\mathbf{r}}^2$  (with the notation  $\langle \dots \rangle_{\mathbf{r}}$  we indicate a spatial average over a macroscopic hypercubic box of linear size  $L$  over the  $d$ -dimensional substrate) characterize the universality class of the model. More precisely, for a system of size  $L$ ,  $w_2(L, t) \sim L^{2\chi} f(t/L^z)$ , where the scaling function is such that  $f(x) \rightarrow \text{const}$  for  $x \rightarrow \infty$  and  $f(x) \sim x^{2\chi/z}$  for  $x \rightarrow 0$ . The peculiar behavior of  $f$  imply that  $w_2(L, t) \sim L^{2\chi}$  for  $t \gg L^z$  and  $w_2(L, t) \sim t^{2\chi/z}$  for  $t \ll L^z$ . Due to an infinitesimal tilt symmetry of Eq. (1) ( $h \rightarrow h + \mathbf{r} \cdot \boldsymbol{\epsilon}$ ,  $\mathbf{r} \rightarrow \mathbf{r} - \lambda t \boldsymbol{\epsilon}$ ), the two critical exponents are related by the scaling relation  $\chi + z = 2$ , which is believed to be valid at any dimension  $d$  [2].

A complete understanding of Eq. (1), and in particular the determination of the two critical exponents  $\chi, z$  for any spatial dimension  $d > 1$  (at  $d = 1$  a fluctuation-dissipation theorem leads to the exact result  $\chi = 1/2$ ,  $z = 3/2$ ), turns out to be extremely difficult for two main reasons: (i) we are dealing with an intrinsically out-of-equilibrium phenomenon where the standard equilibrium toolbox must be used with care, (ii) perturbative renormalization schemes are not adequate for describing the strong coupling regime (*i.e.* where the parameter  $\lambda$  is relevant).

The existence of an upper critical dimension  $d_u$ , *i.e.* the substrate dimensionality  $d$  above which the fluctuation of the model become irrelevant ( $\chi = 0$ ), is one of the most controversial unsolved theoretical issues related with Eq. (1). The determination of  $d_u$  would be a most relevant achievement since, as customary in equilibrium critical phenomena, its knowledge constitutes the first step for a controlled perturbative expansion around it. The quest for  $d_u$  has been around for more than twenty years [3–15] and the different predictions range from  $d_u \approx 2.8$  to  $d_u = \infty$ . Analytical estimates using the mode-coupling theory yield exact results in  $d = 1$  [16]. Their extension to higher dimensions hints for a  $d_u = 4$  under different self-consistency schemes [5–9]. The same value for  $d_u$  is also supported by different field-theoretic approaches [3, 10–12].

At odd with what predicted by the previously mentioned field-theoretic approaches, both direct numerical integration of KPZ equation [17], and simulation of systems belonging to the KPZ universality class [13, 14, 18, 19] indicate that  $d_u > 4$ , while the real-space renormalization group approach [15] predicts  $d_u = \infty$ .

Such a long standing controversy is the consequence of the difficulties inherent to both analytical and numerical approaches. Most of the assumptions made on the functional structure of the sought solution in the different field-theoretic analysis, as well as the approximations made in the mode-coupling theories are, in general, not completely under control. On the numerical side the most severe problem is due to the fact that simulations in high spatial dimensions  $d \geq 4$  are computationally very heavy, and the systems under analysis must be limited in size. As a consequence, the different fitting procedures must deal with controlled finite-size scaling procedures to yield reliable estimates of the critical exponents. Under this perspective, particularly relevant is the observation that for lattice models in the KPZ universality class, a controlled asymptotic regime is achieved only when typical scale of the fluctuations is larger than the lattice spacing used in the simulations or, more precisely, for  $w_2 > 1$  [9]. The former inequality is very stringent from the computational point of view since it requires very large lattices to be fulfilled: the estimates presented in [14] suggest indeed that for the 4-dimensional RSOS model, to which this letter is addressed, the  $w_2 > 1$  inequality starts being verified for lattice size larger then  $L \approx 32$ , whereas the larger system size analyzed in the same paper was  $L = 28$  that, at the best of our knowledge, remains the larger system in 4 dimensions simulated so far.

To settle the controversy, at least in the 4-dimensional RSOS model case, we decided to analyze samples of unprecedented size: we have been able investigate the steady state scaling regime  $t \gg L^z$  for lattice size volumes up to  $V = 128^4 = 268435456$  sites, a factor 437 off the largest simulation known in literature [14]. We can also study the dynamic scaling regime of lattices of  $V = 256^4 = 4294967296$  sites, but for such a large size we have been able to investigate the asymptotic scaling regime for just three samples, due to limitations in our computing facility (most of the data for  $L = 256$  are at not too large  $t$  and they have been used only in fig. (1): they appear only in the region  $t/L^z < 8$ ).

The RSOS can be simulated in the following way: at any time  $t$  we randomly select a site  $i$  on the  $d$ -dimensional lattice and we let the surface height  $h_i$  at that point to grow of a unit  $h_i(t+1) = h_i(t) + 1$  only if  $\max_{j \in \partial i} |h_i(t) - h_j(t)| \leq 1$ , being  $\partial_i$  the set of 8 nearest neighbors of  $i$  in  $d = 4$  (note that we will assume periodic boundary conditions).

We simulated RSOS growth using two different algorithms based on a very efficient *multi-spin coding* technique [20] originally developed for disordered spin system, and later generalized to deal with the RSOS model [14]:

- *Multi Surface (MS) coding*: we can simulate, with basically the same cost of one single surface simulation,  $N_b$  copies of the system,  $N_b$  being the number of bits in a computer word (usually 32, 64, 128 and 256). We transform the basic operations (like summing spins for computing the effective force) into Boolean operations, and we exploit the fact that when, for instance, the computer is calculating an AND logical bit, it is indeed doing that operation  $N_b$  times at once, i.e. for all the bits of the world. Unfortunately computational efficacy of this method is counterbalanced by the memory load, making it unpractical for analyzing samples of linear size larger than  $L = 64$ , at least on the computers we have access to.
- *Multi Lattice-site (ML) coding*: for sample of linear size  $L = 128, 256$  we have developed a new multi-spin coding representation in which a single surface at time is simulated, but we lump together  $N_b$  height-difference local variable in a single computer word of  $N_b$  bits. We will refer to this second method as the Multiple Lattice-site (ML) algorithm (see table I). In this algorithm in the first half step we update the even spins (i.e. the spins  $\sigma_i$  where  $i_x + i_y + i_z + i_t$  is even) applying the standard RSOS procedure with probability 1/2 to each spin (with probability 1/2 the spin is not updated), in the second half step we apply the algorithm to odd spins. Some programming care must be used with periodic boundary conditions: in the simplest version we have used,  $L$  must be an even multiple of  $N_b$ . Moreover it is crucial to use a good random number generator, where *all* the bits are random.

$L$	sweeps	samples	type	time (h.)
8	524000	1024	MS	4
16	524000	1024	MS	6
31	524000	1024	MS	121
32	524000	1024	MS	139
33	524000	1024	MS	158
64	131000	512	MS	5376
128	512000	64	ML	7680
256	130000	64	ML	504

TABLE I. In this table we display the lattice linear size  $L$ , the number of montecarlo sweeps (full lattice update), the number of samples and the simulation type (MS = multi-surface coding, ML = multi-lattice coding), and the overall computational time in hours.

We simulate 4-dimensional lattices of volume  $V = L^4$  for lattices of linear size  $L = 8, 16, 31, 32, 33, 64, 128$ . For the two largest lattice ( $L = 64, 128$ ) we run the ML algorithm, while for the rest we run the MS algorithm. We decided to consider  $L = 31, 33$  for checking that there are no periodicity issues with the random number generator. A summary of our simulations is provided in table I.

	$\chi$	$\omega$	$A_2$	$B_2$	$A_3$	$B_3$	$A_4$	$B_4$
NEW	0.2537(8)	1.11(9)	0.171(1)	0.37(6)	0.0319(3)	-1.0(2)	0.100(1)	0.38(8)
OLD	0.255(3)	0.98(9)	0.170(1)	0.37(3)	0.0321(2)	-0.7(1)	0.100(1)	0.46(4)

TABLE II. In this table we display the best fit values together with their statistical error of the parameters defined in Eq. (4). The first row refers to the actual data presented in this work, the second is taken from [14]

The simulations aim at achieving a fair sampling of the asymptotic regime. To do so, at any time  $t$  and for each sample (both in ML and MS type of simulation) we evaluate the first three connected moments  $w_n(L, t) = \sum_{i=1}^V (h_i(t) - \langle h(t) \rangle)^n / V$ , where  $\langle h(t) \rangle = \sum_{i=1}^V h_i(t) / V$ , and  $n = 2, 3, 4$ . We thus define our asymptotic (in time) estimate as:

$$w_n(L) = \frac{1}{T_0 - T_1 + 1} \sum_{t=T_1}^{T_0} w_n(L, t) \quad . \quad (3)$$

We are careful to choose both  $T_0$ , and  $T_1 - T_0$  large enough to guarantee: (i) convergence to the asymptotic regime, i.e. that  $T_1 \gg L^z$ , (ii) a large enough sampling of statistically uncorrelated measures of  $w_n(L, t)$ . In practice we consider consecutive measuring windows of length 64, 128, ...,  $T_1, T_0$ , so that  $T_0$  is the last measure in the simulation and  $T_1 = T_0/2$ . This choice is

very conservative, since eventually we use just the second half of the simulation, but at the same time it allows us to check with very high reliability whether or not we have reached the asymptotic state: a quick look at Fig. 1 will comfort our confidence of having chosen, even for the larger sample size, a  $T_0 \gg L^z$ , at least of a factor 100 off. We are now ready to determine the critical exponents of the asymptotic behavior of  $w_n$ , which scales as  $L^{n\chi}$  at the leading order, by fitting simultaneously the following moments:

$$\begin{aligned} w_2 &= A_2 L^{2\chi} (1 + B_2 L^{-\omega}) \\ w_3 &= A_3 L^{3\chi} (1 + B_3 L^{-\omega}) \\ w_4 &= A_4 L^{4\chi} (1 + B_4 L^{-\omega}) \end{aligned} \quad (4)$$

where  $\omega$  is the leading finite size scaling exponent. The fit involves the simultaneous determination of 8 parameters whose best-fit value is reported in the first row of table II (the fit yields a chi-squared root mean square deviation of 2.05). Interestingly enough the fit presented in [14] agrees very well with the new data as we can clearly appreciate qualitatively in Fig. 2, and more quantitatively by comparing the two rows in table II. With respect to the  $w_2 > 1$  inequality issue, a glance at Fig. 2 shows unambiguously that the scale of the typical fluctuations, for all lattice size larger than  $L = 31$ , verify the inequality. We do not see any change in the scaling behavior of the three cumulants around the cross-over region  $L \approx 30$ , moreover, the fact that the old fit presented in [14] (in a regime  $w_2 < 1$ ) agrees so well with our larger lattice size simulation (see again Fig. 2) indicate that the simulations performed for  $L \leq 28$  were able to capture fairly the asymptotic scaling regime. To see more clearly the finite-size corrections of  $\chi$  we determined the effective exponent  $\chi_n^{\text{eff}}$  as the discretized logarithmic derivative of Eqs. (4) which in our case reads:

$$\chi_n^{\text{eff}}(L) = \frac{\log(\frac{w_n(L)}{w_n(L')})}{n \log(\frac{L}{L'})} \quad (5)$$

where  $L/L' = 2$ , and  $n = 1, 2, 3$ . In Fig. 3 we display  $\chi_n^{\text{eff}}$  as a function of  $L^{-1}$  (note that we discarded for the sake of clarity the  $L = 31, 33$  results) for the three cumulants together with the best-fit curves. The fit yields the following results for the critical exponents:  $\chi = 0.2532(5)$  and  $\omega = 1.14(5)$  (see also table II).

A recent has investigated a model of direct polymers in random medium that should belong to the same universality class [18]. In this model one can define an exponent  $\zeta$  that according to the theoretical expectations should be given

$$\zeta = \frac{1}{2 - \chi} \quad (6)$$

Their results ( $\zeta$  slightly larger than 0.57), is well consistent with our prediction  $\zeta = 0.5725(2)$ .

The numerical technique we have introduced has allowed us to run very precise numerical simulations of the RSOS model in  $d = 4$  on unprecedented system size with a limited amount of computational time. Thanks to the accuracy of the simultaneous measurement of the three cumulants, the claim that  $d = 4$  is the upper critical dimension for systems in the KPZ universality class has to be rejected. Moreover, the typical fluctuation's length-scale of our simulations on samples of linear size  $L = 128$  and  $L = 256$  are larger than the lattice spacing, and this is a clear indication that: (i) the system reached a controlled scaling regime, (ii) the measured scaling exponents are reliable and not affected by a pre-asymptotic cross-over regime.

There is still a remote possibility that our data are consistent with an upper critical dimension  $d_u = 4$  of the KPZ equation if we drop the hypothesis that RSOS in  $d = 4$  belongs to the KPZ universality class. However, apart from some work in the past [21], this hypothesis does not seem to have support in the mainstream literature on KPZ.

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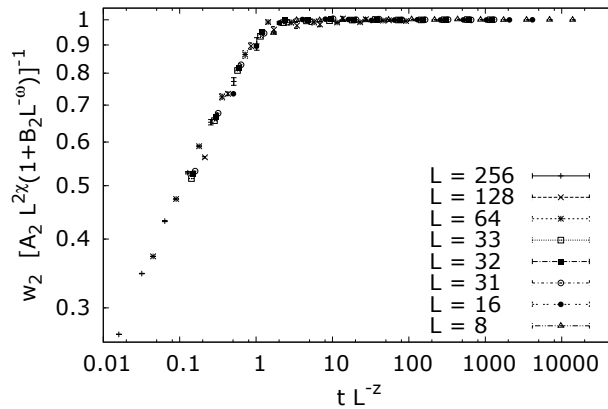


FIG. 1. Scaling plot of the rescaled second moment  $w_2 / (A_2 L^{2\chi} (1 + B_2 L^{-\omega}))$  vs. the rescaled time  $t / L^z$ .

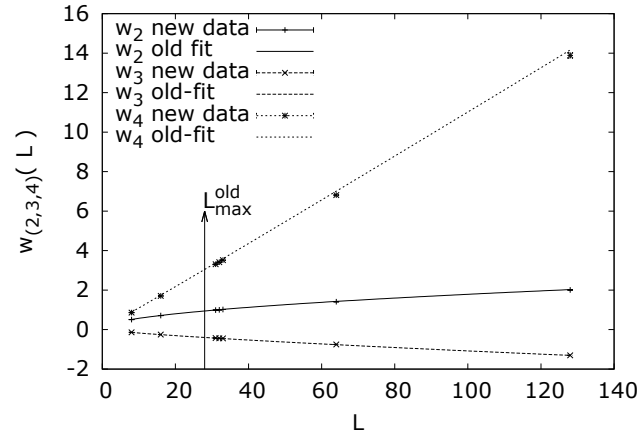


FIG. 2. The quantities  $w_2$ ,  $w_3$ ,  $w_4$  are displayed as a function of  $L$ . Dots with error bars are values obtained by simulations, while solid lines are the 8-parameters best-fit reported in [14]. The vertical arrow at  $L = 28$  represents the largest size simulated in [14].

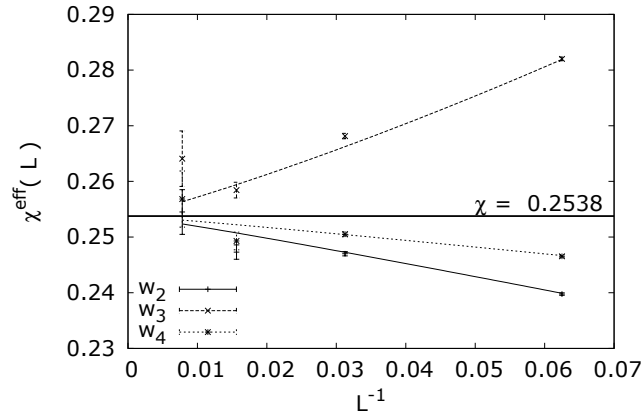


FIG. 3. Local slopes of  $w_{2,3,4}$  are displayed as a function of  $L^{-1}$ . Dots with error bars are values obtained by simulations, while lines are the 8-parameters best-fit reported in table II. The solid horizontal line is at  $\chi = 0.2538$ , i.e. the best-fit prediction for the wandering exponent.